

cosmoabc: Likelihood-free inference via Population Monte Carlo Approximate Bayesian Computation

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Abstract

Approximate Bayesian Computation (ABC) enables parameter inference for complex physical systems in cases where the true likelihood function is unknown, unavailable, or computationally too expensive. It relies on the forward simulation of mock data and comparison between observed and synthetic catalogues. Here we present COSMOABC, a Python ABC sampler featuring a *Population Monte Carlo* variation of the original ABC algorithm, which uses an adaptive importance sampling scheme. The code is very flexible and can be easily coupled to an external simulator, while allowing to incorporate arbitrary distance and prior functions. As an example of practical application, we coupled COSMOABC with the NUMCOSMO library and demonstrate how it can be used to estimate posterior probability distributions over cosmological parameters based on measurements of galaxy clusters number counts without computing the likelihood function. COSMOABC is published under the GPLv3 license on PyPI and GitHub and documentation is available at <http://goo.gl/SmB8EX>.

1. Introduction

The precision era of cosmology marks the transition from a data-deprived field to a data-driven science on which statistical methods play a central role. The ever-increasing data deluge must be tackled with

new and innovative statistical methods in order to improve our understanding of the key ingredients driving our Universe (e.g., Borne, 2009; Ball & Brunner, 2010; de Souza et al., 2014; de Souza & Ciardi, 2015). Given the continuous inflow of new data, one does not start an analysis from scratch for every new

telescope, but is guided by previous knowledge accumulated through experience. A new experiment provides extra information which needs to be incorporated into the larger picture, representing a small update on the previous body of knowledge. Such a learning process is a canonical scenario to be embedded in a Bayesian framework, which allow us to update our degree of belief on a set of model parameters¹ whenever new and independent data are acquired.

A standard Bayesian analysis specifies prior distributions on unknown parameters, defines which parameter values better describe the relationship between the model, the prior and the new data, and then finds the posterior distribution – either analytically or via sampling techniques, as e.g. with Markov Chain Monte Carlo (MCMC; Metropolis et al., 1953). This analysis requires a proper construction of the likelihood function, which is not always well known or easy to handle. A common solution would be to construct a model for the likelihood (e.g. a Gaussian) followed by MCMC, with the expectation that this hypothesis is not too far from the true. Nonetheless, the challenge of performing parameter inference from an unknown or intractable likelihood function is becoming familiar to the modern astronomer. Recent efforts to overcome observational selection biases in the study of massive (Sana et al., 2012) and not-so massive (Janson et al., 2014) stars, to account for windowing effects, errors and/or gaps in time-series of X-ray emission from active galactic nuclei (Uttley et al., 2002; Shimizu & Mushotzky, 2013) and UV emission from stellar coronae (Kashyap et al., 2002) have been reported.

The development of *ad hoc* approaches to this problem within astronomy have proceeded independently from their long history within the field of population genetics. The latter have ultimately been formalized into a rigorous statistical technique known as Approximate Bayesian Computation (ABC). The

intuition of ABC dates back to a thought-experiment in Rubin (1984), where the basic ABC rejection sampler is used to illustrate Bayes Theorem. Tavaré et al. (1997) employs an acceptance-rejection method in the context of population genetics, while Pritchard et al. (1999) presents the first implementation of a basic ABC algorithm. Only recently has the ABC approach been introduced and applied to astronomical problems (Cameron & Pettitt, 2012; Schafer & Freeman, 2012; Weyant et al., 2013; Robin et al., 2014). This work is part of a larger endeavour natural consequence of such initial efforts. Following the philosophy behind the *Cosmostatistics Initiative* (COIN)², we present a tool which enables astronomers to easily introduce ABC techniques into their daily research.

The cornerstone of the ABC approach is our capability of performing quick and reliable computer simulations which mimic the observed data in the best possible way (this is called *forward simulation inference*). In this context, our task relies on performing a large number of simulations and quantifying the “distance” between the simulated and observed catalogues. The better a parametrization reproduces the observed data in a simulated context, the closer it is to the “true” model. From this simple reasoning, many alternatives were developed to optimize the parameter space sampling and the definition of distance. One of such examples is the work of Marjoram et al. (2003), who proposes a merger between the standard MCMC algorithm and the ABC rejection sampling. In astronomy, the method was used by Robin et al. (2014) to constrain the Milky Way thick disk formation. Going one step further, Beaumont et al. (2009a) propose to evolve an initial set of parameter values (or *particle system*) through incremental approximations to the true posterior distribution. The *Population Monte Carlo ABC* (PMC-ABC), method was used to make inferences on rate of morphological transformation of galaxies at high redshift (Cameron & Pettitt, 2012) and proved to be efficient in tracking the Hubble parameter evolution from type Ia supernova measurements, despite the contamination from type II supernova (Weyant et al., 2013). More recently, Lin & Kilbinger (2015) used ABC to predict weak lensing peak counts and Killedar

¹For the purposes of this work, we will only be interested in the *parameter values* of a given model. However, it is important to stress that in a completely Bayesian approach all the elements and hypotheses forming the model can be considered part of the *prior*. In this sense, with the arrival of new essential information, the Bayesian approach allows for completely redefinition of the model itself (Kruschke, 2011).

²<http://goo.gl/rQZSAB>

et al. (2015) applied a weighted variant of the algorithm to cluster strong lensing cosmology.

This work introduces `cosmoabc`³, the first publicly available⁴ Python ABC package for astronomy⁵. The package is structured so that the simulation, priors and distance functions are given as input to the main PMC-ABC sampler. In this context, users can easily connect the ABC algorithm to their own simulator and verify the effectiveness of the tool in their own astronomical problems. The package also contains exploratory tools which help defining a meaningful distance function and consequently point to appropriate choices before the sampler itself is initiated.

We first guide the user through a very simple toy model, in order to clarify how the algorithm and the package work. Subsequently, as an example of cosmological application, we show how the machinery can be used to define credible intervals over cosmological parameters based on galaxy clusters catalogues. Simulations for this example were performed using the *Numerical Cosmology* library (`NUMCOSMO`; Vitenti & Penna-Lima, 2014). The connection between `cosmoabc` and `NUMCOSMO` is implemented as an independent module that can be easily adapted to other cosmological probes.

The outline of this article is as follows. In section 2, we give an overview of Bayesian perspective and the ABC algorithm. `cosmoabc` package is presented in section 3 through a simple toy model. Section 4 describes in detail how to connect `cosmoabc` and `NUMCOSMO` to obtain constraints over cosmological parameters from galaxy cluster number counts. Our final remarks are presented in section 5.

2. Bayesian approaches to parameter inference

Statistical inference on unknown parameters is often a primary goal of a physical experiment design. Although it is possible, and at times even desirable, to encounter some unpredictable behaviour

among the outcomes of an experiment or a measurement, in many situations the experimentation aims at establishing constraints over the parameters of a model. In other words, the desire is to use real-world data to check prevailing theories.

In the Bayesian framework, the data are seen as the accessible truth regarding a given physical process and the model as a representation of our understanding of such process. This approach is data-centred and allows us to update the model whenever new information becomes available. In other words, our goal is to determine the probability of a model given the data,

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})}, \quad (1)$$

where θ is the vector of model parameters, \mathcal{D} the data set, $p(\theta|\mathcal{D})$ is called the *posterior*, the prior, $p(\theta)$, represents our initial expectations towards the model and $p(\mathcal{D})$ is a normalization constant.

In this context, the model parameters themselves are considered random variables and each individual measurement corresponds to one realization of them. Thus, once our prior is confronted with the data, the outcome is a posterior probability distribution function (PDF). Using the posterior distributions we can determine *credible intervals*, which represent our uncertainty about the model parameters⁶. For example, one may be interested in the most-probable region of values for certain parameters.

2.1. Approximate Bayesian Computation

The ABC algorithm uses our ability to simulate the physical process under investigation to bypass the necessity of an unknown or computationally too expensive likelihood function. It is based on the following crucial elements:

- a simulator, or forward model,
- prior probability distributions over the input parameters $p(\theta)$,

³<https://pypi.python.org/pypi/CosmoABC>

⁴Shortly after `cosmoabc` was released Akeret et al. (2015) also presented a Python package for forward modelling through PMC-ABC.

⁵For similar tools in the context of biology and genetics, see e.g. Liepe et al. (2010); Oaks (2014).

⁶Not to be confused with the frequentist definition *confidence interval*, where the parameter values are considered fixed and therefore, there is no probabilistic interpretation associated to them.

- a distance function, $\rho(\mathcal{D}_1, \mathcal{D}_2)$.

As a simple example, consider the following toy model: a given physical process can be probed through a catalogue of P observations, $\mathcal{D} = \{x_i, \dots, x_P\}$. Our model states that this process is driven by a random variable, X , following a Gaussian distribution, $X \sim \mathcal{N}(\mu_0, \sigma_0)$. Thus our goal is to identify credible intervals over μ_0 and σ_0 based on \mathcal{D} . Moreover, our prior states that $\mu_0 \in [\mu_-, \mu_+]$ and $\sigma_0 \in [\sigma_-, \sigma_+]$. Hereafter, we will denote the model parameters as $\theta = \{\mu, \sigma\}$.

The main idea behind the ABC algorithm can be summarized in three main steps:

- draw a large number of parameter values, θ^i , from the prior distribution, p ,
- for each θ^i generate a simulation, \mathcal{D}_S^i , and calculate the distance between the observed to the simulated catalogues, $\rho^i = \rho(\mathcal{D}, \mathcal{D}_S^i)$,
- approximate the posterior probability distribution using the fraction of θ^i 's with smallest associated distances.

The above method has been modified and further developed in the last decade, generating some alternatives to the main algorithm (e.g. Sisson et al. 2007; Drovandi & Pettitt 2011; Marin et al. 2012; Del Moral et al. 2012; Ratmann et al. 2013). One of them is presented below.

2.2. Distance

In the toy model described above, we can safely determine the distance, ρ , between the measured catalogue \mathcal{D} and a simulated one \mathcal{D}_S as

$$\rho = \text{abs}\left(\frac{\bar{\mathcal{D}} - \bar{\mathcal{D}}_S}{\bar{\mathcal{D}}}\right) + \text{abs}\left(\frac{\sigma_{\mathcal{D}} - \sigma_{\mathcal{D}_S}}{\sigma_{\mathcal{D}}}\right), \quad (2)$$

where $\bar{\mathcal{D}}$ is the mean of all measurements in catalogue \mathcal{D} and $\sigma_{\mathcal{D}}$ is its standard deviation. Equation 2 encloses important properties, which should be present in any ABC distance function: the distance between two identical catalogues is zero and the distance value increases steeply as parameter values get further from the fiducial ones. We emphasize that the choice of the distance function is a crucial step in

Table 1: Glossary for algorithm 1.

Parameter	Description
\mathcal{D}	Observed data set
\mathcal{D}_S	Simulated catalogue
M	Number of draws for the first iteration
\mathcal{S}	Particle system
N	Number of particles in \mathcal{S}
t	Time-step (iteration) index
K	Number of draws index
W	Importance weights
ϵ	Distance threshold
Δ	Convergence criterion
θ	Vector of model parameters
$p(\cdot)$	Prior distribution
$\rho(\cdot, \cdot)$	Distance function
$\mathcal{N}(\bullet; \theta, C)$	Gaussian PDF at \bullet with $\mu = \theta$, cov= C

the design of the ABC algorithm and the reader must check its properties carefully before any ABC implementation is attempted.

2.3. Population Monte Carlo ABC

COSMOABC uses the algorithm proposed by Beaumont et al. (2009a), where successive steps towards the posterior are achieved by applying an importance (or weighted) sampling in the set of parameter values whose distances satisfy a given initial threshold.

We begin by drawing M values from the prior, called *particles*, $\{\theta^i\}$ with $i \in [1, M]$, such that $M \gg N$ (N is the number of samples needed to characterize the prior). For each particle we generate a forward model (simulation) and calculate the distance between synthetic and real catalogues $\rho^i = \rho(\mathcal{D}, \mathcal{D}_S^i)$. From this large set, we keep only the N particles with smallest ρ^i , which constitute the first *particle system* ($\mathcal{S}_{t=0}$) and determine a distance threshold for the next iteration ($\epsilon_{t=1}$) as the 75% quantile of all $\rho \in \mathcal{S}_{t=0}$. In this initial step, we associate to each particle the same weight, $W_{t=0}^j = 1.0/N$, for $j \in [1, N]$.

In subsequent iterations, $t > 0$, we perform an *importance sampling* from \mathcal{S}_{t-1} : a popular technique where one can draw from a proposal distribution and re-weight the particle system so it targets the desired posterior distribution.

Data: $\mathcal{D} \rightarrow$ observed catalogue.

Result: ABC-posteriors distributions over the model parameters.

```

 $t \leftarrow 0$ 
 $K \leftarrow M$ 
for  $J = 1, \dots, M$  do
    Draw  $\theta$ , from the prior,  $p(\theta)$ .
    Use  $\theta$  to generate  $\mathcal{D}_S$ .
    Calculate distance,  $\rho = \rho(\mathcal{D}_S, \mathcal{D})$ .
    Store parameter and distance values,
         $\mathcal{S}_{\text{ini}} \leftarrow \{\theta, \rho\}$ 
end
Sort elements in  $\mathcal{S}_{\text{ini}}$  by  $|\rho|$ .
Keep only the  $N$  parameter values with lower
distance in  $\mathcal{S}_{t=0}$ .
 $C_{t=0} \leftarrow$  covariance matrix from  $\mathcal{S}_{t=0}$ 
for  $L = 1, \dots, N$  do
     $W_1^L \leftarrow 1/N$ 
end
while  $N/K > \Delta$  do
     $K \leftarrow 0$ .
     $K_* \leftarrow 0$ .
     $t \leftarrow t + 1$ .
     $\mathcal{S}_t \leftarrow []$ .
     $\epsilon_t \leftarrow 75^{\text{th}}$ -quantile of distances in  $\mathcal{S}_{t-1}$ .
    while  $\text{len}(\mathcal{S}_t) < N$  do
         $K_* \leftarrow K_* + 1$ 
        Draw  $\theta_0$  from  $\mathcal{S}_{t-1}$  with weights  $\bar{W}_{t-1}$ .
        Draw  $\theta$ , from  $\mathcal{N}(\theta_0, C_{t-1})$ .
        Use  $\theta$  to generate  $\mathcal{D}_S$ .
        Calculate distance,  $\rho = \rho(\mathcal{D}_S, \mathcal{D})$ 
        if  $\rho \leq \epsilon_t$  then
             $\mathcal{S}_t \leftarrow \{\theta, \rho, K_*\}$ 
             $K \leftarrow K + K_*$ 
             $K_* \leftarrow 0$ 
        end
    end
for  $J = 1, \dots, N$  do
     $\tilde{W}_t^J \leftarrow$  equation (3).
end
 $W_t \leftarrow$  normalized weights.
 $C_t \leftarrow$  weighted covariance matrix from
 $\{\mathcal{S}_t, W_t\}$ .
end

```

Algorithm 1: PMC-ABC algorithm implemented in COSMOABC.

The parameter vector resulting from this importance sampling, θ_{try} , is used to simulate a catalogue and calculate its distance to the observed data, ρ_{try} . The parameter θ_{try} is stored if $\rho_{\text{try}} \leq \epsilon_t$. This process is repeated until a new set of N parameter values satisfying the distance threshold is completed. For the new particle system, the weights are calculated as

$$W_t^j = \frac{p(\theta_t^j)}{\sum_{i=1}^N W_{t-1}^i \mathcal{N}(\theta_t^j; \theta_{t-1}^i, C_{t-1})}, \quad (3)$$

where W_t^j denotes the weight associated to the j -th particle in particle system t , $p(\theta_t^j)$ corresponds to the prior probability distribution calculated at θ_t^j , W_{t-1}^i is the weight of the i -th particle in particle system $t-1$ and $\mathcal{N}(\theta_t^j; \theta_{t-1}^i, C_{t-1})$ represents a Gaussian PDF⁷ centred in θ_{t-1}^i , with covariance matrix built from \mathcal{S}_{t-1} and calculated at θ_t^j .

Once the new weights are determined, we start the construction of a new particle system and the algorithm is repeated until convergence. As pointed out by Beaumont et al. (2009b), this is achieved when the ABC posterior no longer changes substantially with subsequent iterations. Here we consider that the system converged when the number of draws necessary to construct a particle system is much larger than N (see algorithm 1 and Section 3.2). Each iteration brings us closer to the “true” PDF bypassing the need of a full likelihood calculation. Moreover, as the calculation of one particle is independent from the others within each iteration, the algorithm itself is more easily parallelizable than a standard MCMC.

3. COSMOABC

In COSMOABC, our toy model can be represented by a simulation function,

```

1 from scipy.stats import norm
2 import numpy as np
3
4 def my_simulation(v):
5     """ Toy model simulator """
6

```

⁷In general, the Gaussian PDF works well, but can be replaced with a different distribution if the parameter space has special restrictions, e.g. only takes integer values.

```

7     dist = norm(loc=v['mean'],
8                 scale=v['std'])
9     l1 = dist.rvs(size=v['n'])
10
11     return np.atleast_2d(l1).T

```

where v is a dictionary of input parameters whose keywords `mean` and `std` determine the mean and standard deviation of the underlying Gaussian distribution, respectively, and `n` denotes the total number of objects in the catalogue. Analogously, a flat prior would be written as⁸

```

1 from scipy.stats import uniform
2
3 def my_prior(par, func=False):
4     """Flat prior"""
5
6     gap = par['pmax'] - par['pmin']
7     pdf = uniform(loc=par['pmin'],
8                  scale=gap)
9     if func == False:
10         draw = pdf.rvs()
11         return draw
12     else:
13         return pdf

```

with `par` as a dictionary of input parameters and the keys `pmin` and `pmax` determining the boundaries of the distribution.

The distance function should be written as

```

1 import numpy as np
2
3 def my_distance(d2, p):
4     """Distance function."""
5
6     dmean = np.mean(p['dataset1']) -
7              np.mean(d2)
8     dstd = np.std(p['dataset1']) -
9            np.std(d2)
10
11     gmean = abs(dmean/
12                np.mean(p['dataset1']))
13     gstd = abs(dstd/
14               np.std(p['dataset1']))
15
16     rho = gmean + gstd
17
18     return np.atleast_1d(rho)

```

⁸The `func` argument is needed so we can retrieve a realization and the probability distribution itself. This is used by COSMOABC in the calculation of the weights.

and receive as input the simulated catalogue `d2` and the dictionary `p`. Notice that the observed catalogue is contained in `p`. So the distance to be calculated is between `p['dataset1']` and `d2`⁹.

We must store these three functions in one file, `<func_file>`, and edit the sample input file provided within COSMOABC. Each keyword in the sample input file is self-explanatory, so here we only emphasize the model and prior function parameters

```

1 param_to_fit = mean std
2 param_to_sim = mean std n
3
4 mean_prior_par_name = pmin pmax
5 mean_prior_par_val = -2.0 4.0
6
7 std_prior_par_name = pmin pmax
8 std_prior_par_val = 0.1 5.0
9
10 mean_lim = -2.0 4.0
11 std_lim = 0.1 5.0
12
13 mean = 2.0
14 std = 1.0
15 n = 1000
16 ...
17 prior_func = my_prior my_prior

```

Notice that although the variables `mean` and `std` are free parameters, we need to provide an initial numerical value, within the constraints allowed by the prior. The parameter `prior_func` stores the prior PDF for all the free parameters, in the sequence declared in the variable `param_to_fit`. Such priors do not need to follow the same family of distribution. It is possible to define a flat prior for the first parameter and a Gaussian one for the second. In that case the user input file would include, for example,

```

1 mean_prior_par_name = pmin pmax
2 ...
3 std_prior_par_name = pmean pstd
4 ...
5 ...
6
7 prior_func = my_prior gaussian_prior

```

considering `pmean` and `pstd` as the mean and stan-

⁹This format was chosen in order to optimize parallelization.

dard deviation for the Gaussian prior the second parameter under investigation.

3.1. Visualizing distance behaviour

Before we attempt to use the ABC sampler, it is important to have an idea of how our distance definition behaves for different combination of model parameter values. COSMOABC has a tool which allows us to visually inspect the performance of our distance definition. The code randomly selects parameter values from the prior, performs the simulation and calculates the distance for each one of them. These distances are then plotted as a function of the parameter values, one parameter at a time. Ideally, the scatter of points in the $\rho \times \theta$ space should present a clear minimum in the neighbourhood of the most likely parameter value.

In order to test a personalized distance function, do

```
1 $ test_ABC_distance.py -i <input_file>
2                        -f <func_file>
```

An example of the result of this test for the toy model we have been considering is shown in Figure 1. Notice that the distance behaves as expected, approaching zero around the fiducial values $\text{mean}=2.0$ and $\text{std}=1.0$ and rapidly increasing as parameter values move further away.

It is worth mentioning that this procedure was implemented only to provide the user with an intuition regarding the distance function dependence with model parameters. The behaviour illustrated in Figure 1 is a necessary but not sufficient characteristic of an ideal diagnostic. Selecting an appropriate distance function is an open and problem dependent challenge but it is an active area of statistical research (see e.g. Fearnhead & Prangle, 2012; Blum et al., 2013; Ratmann et al., 2013). A deeper investigation on the steps leading to an optimal distance definition, although very important, is out of the scope of this work.

3.2. Running the ABC sampler

After we are convinced of the performance of our distance function, we can proceed to the ABC sampler run. In COSMOABC, this is done through

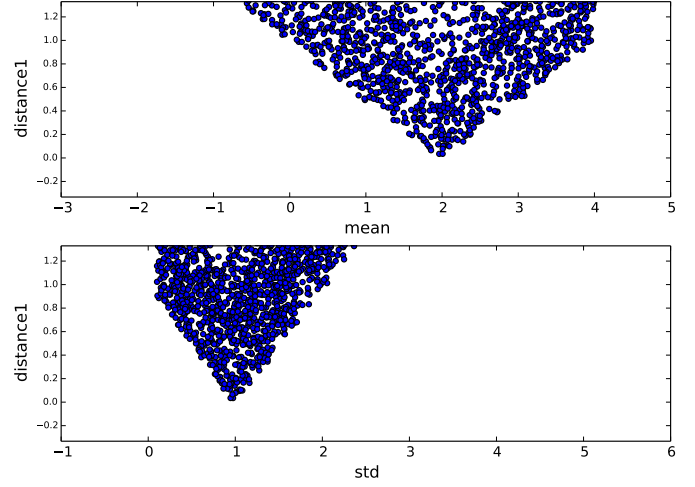


Figure 1: Behaviour of the distance function proposed in our toy model as a function of the free parameters mean (top) and std (bottom).

```
1 $ run_ABC.py -i <input_file>
2              -f <func_file>
```

The time necessary for the algorithm to converge depends on the efficiency of the simulator, the behaviour of the distance function and the number of particles in each particle system. We suggest an initial run with a fairly large convergence threshold, for example $\text{delta} = 0.25$. This means that the code will run until it is necessary to take 4 times more draws than the number of particles in each particle system. In order to facilitate debugging and interaction with other codes, for each particle system COSMOABC outputs parameter values, distance, distance threshold, computational time and weights for each particle in ASCII tables.

Once the algorithm converges, it is possible to visualize the results with

```
1 $ plot_ABC.py -i <input_file>
2              -f <func_file>
3              -p T
```

This will generate a file containing one snapshot for each particle system from $t=0$ to $t=T$, as well as plots for the evolution of distance threshold, convergence criteria and computational time. From this first quick test, the user can either be satisfied with the achieved result or decide to continue iterating the sampler. If more iterations are required, it is only necessary to decrease the parameter delta in the user input file

and continue from the last completed particle system

```
1 $continue_ABC.py -i <input_file>
2                  -f <func_file>
3                  -p T
```

4. Case study: cosmological parameter inference from Sunyaev-Zeldovich surveys

The current concordance cosmology has been remarkably successful in explaining the observed properties of large-scale structures (Tegmark et al., 2006; Benson, 2010). In this framework, the formation of such structures proceeds in a hierarchical manner driven by pressureless cold dark matter, where galaxy clusters stand out among the largest bound objects observed so far. The development of an underlying theory of cluster formation (see Kravtsov & Borgani, 2012, for a review), allows us to use the abundance of clusters as well as their spatial distribution as powerful cosmological probes (e.g., Allen et al., 2008).

There are, however, a couple of caveats which make this an interesting problem for the ABC approach: the model is not deterministic, in the sense that it considers the observed data as a realization of a Poisson distribution (analogously to the toy model studied before) and the unavoidable modelling of the observable uncertainties and errors in both, photometric redshifts and mass estimates (for a mathematical description we refer the reader to Appendix A, Penna-Lima et al. (2014) and references therein). Using PMC-ABC surpasses the need to integrate a very complex likelihood function and reduces the influence of initial hypothesis on photometric redshift errors in the estimated posterior PDFs.

Since there is no previous literature on the application of PMC-ABC to this particular problem, it is crucial to establish a proof of concept. Thus, here we present results from a completely synthetic framework, where the “observed” data, \mathcal{D} , is one instance of our forward model. This allows us to provide a controlled scenario and to ensure our capability of recovering the input parameter values. It also facilitates the identification (and quantification) of eventual biases in the final ABC-posteriors.

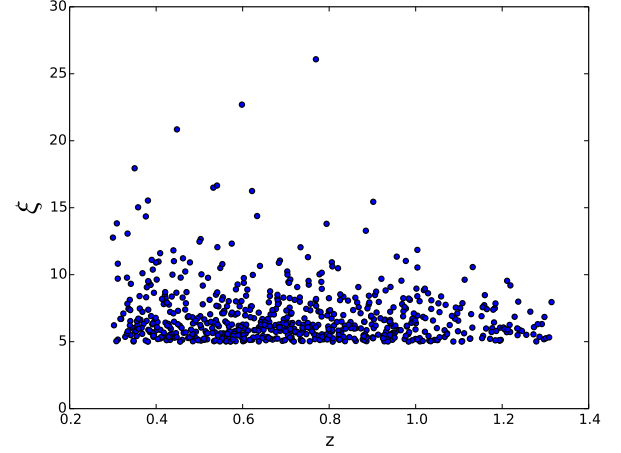


Figure 2: Distribution of observed features (detection significance, ξ , and redshift, z) in the “observed” catalogue, \mathcal{D} .

4.1. Simulations or the forward model

Mock catalogues were generated with the NUMCOSMO library¹⁰, which provides a set of tools to perform cosmological calculations. The software allows a large range of possibilities for input cosmological and astrophysical parameters as well as main survey specifications (see Vitenti & Penna-Lima, 2014, for a more detailed description). Moreover, it can also account for the presence of uncertainties from photometric redshifts and mass-observable relation (hereafter, ξ -mass relation, where ξ is the detection significance) which are crucial for a coherent analysis of galaxy clusters number counts.

Cosmological and astrophysical parameters for the fiducial model were chosen in accordance to Reichardt et al. (2013): $\Omega_c = 0.218$, $\sigma_8 = 0.807$, $w = -1.01$, $\Omega_b = 0.044$, $H_0 = 71.15$ km/s/Mpc, $n_s = 0.97$, $A_{SZ} = 6.24$, $B_{SZ} = 1.33$, $C_{SZ} = 0.83$ and $D_{SZ} = 0.24$ (see Appendix A.1 for definitions). Telescope characteristics follow the SPT design, with minimum and maximum redshifts given by $z_{\min} = 0.3$, $z_{\max} = 1.32$, respectively, and survey area $\Delta\Omega = 2500$ deg² (?).

The simulator begins assuming that the total number of galaxy clusters with $z \in [z_{\min}, z_{\max}]$ and $\xi \in [\xi_{\min}, \infty)$ follows a Poisson distribution. It then generates a realization of this distribution, N_{sim} , and the corresponding catalogue $\{\xi_i, z_i\}$, for $i \in \{1, N_{\text{sim}}\}$ (for

¹⁰<http://www.nongnu.org/numcosmo/>

details in the process see Penna-Lima et al., 2014, appendix B). Here, we investigate the three-dimensional space $\{\Omega_c, \sigma_8, w\}$ with flat initial priors, $\Omega_c \in [0.01, 0.6]$, $\sigma_8 \in [0.5, 1.0]$ and $w \in [-3.0, 0.0]$. All other cosmological parameters are considered known and fixed at the values reported above.

COSMOABC contains a warp of the NUMCOSMO simulator which can be accessed through the user input file keyword

```
1 simulation_func = numcosmo_sim_cluster
```

and an example of the input file with all other options tailored for NUMCOSMO simulations is also provided within the package.

Fig. 2 displays the static simulated catalogue we used as “observed” data in the $\xi \times z$ sample space. The sample is composed by 671 clusters with $z \in [0.30, 1.32]$ and $\xi \in [5, 26]$.

4.2. Distance

The complexity enclosed in the cosmological simulations requires some sophistication in designing the distance function. COSMOABC has two built-in definitions which proved to be effective in the galaxy cluster counts scenario: quantiles and Gaussian radial basis function (GRBF) distances.

The `distance_quantile` function returns a vector ρ , having $L + 1$ dimensions, where L is the number of measured features¹¹. For each feature (column in the catalogue), it calculates a few equally spaced quantiles¹². At every quantile, the values of the cumulative distribution functions (CDF) coming from simulated and observed catalogues are subtracted and the square root of their sum is returned. The last dimension accounts for the variability in the total number of objects. If l is the number of objects in \mathcal{D} and l_S is the number of objects in \mathcal{D}_S , the last element of ρ will be

$$\rho_{-1} = \max \left[\text{abs} \left(1 - \frac{l}{l_S} \right), \text{abs} \left(1 - \frac{l_S}{l} \right) \right]. \quad (4)$$

In the construction of the first particle system, the magnitude of this vector, $|\rho|$, is used to select the set

of N particles with smaller distances. Once the first particle system is constructed, the distance threshold ϵ will also be a $L+1$ -dimensional vector. A new set of parameter values θ will only be accepted to populate the next particle system if it satisfies the 3 distance thresholds independently.

We emphasize that this is only a simple and computationally fast distance definition which proved to be efficient in this synthetic scenario of cosmological inference from galaxy clusters number counts for the illustrative purposes of this work. Whenever using ABC in a real data situation, the user must design a distance function which preserves these features for the problem at hand (e.g., see Section 3.3 of Cameron & Pettitt (2012)).

Figure 3 illustrates the effectiveness of this distance definition in determining the cosmological parameters based on SZ flux measurements. The distance calculations were performed using the COSMOABC tool described in section 3.1, however, in order to make the visualization lighter, we display binned results in all three free parameters. In each panel the horizontal axis was divided in 500 bins and each dot represents the smallest distance found in that bin for 10^4 draws. From Figure 3 we see that the first (comparison of CDF over redshift) and second (comparison of CDF over ξ) distance elements do present a local minimum around the fiducial values for Ω_m and σ_8 , although the behaviour is much lighter than in the previously discussed toy model (Figure 1). The role of the third element (comparison between the total number of objects) is to impose an upper limit on the free parameter values, since this element increases steadily for $\Omega_m \geq 0.28$ and $\sigma_8 \geq 0.86$. We also see that there is little hope in using this distance to constraint w , since there is no significant change in behaviour for the three distance elements.

4.3. Results

Specific tools are also available for the case of a SZ survey using NUMCOSMO. Once all the choices are made in the user input file it is possible to run the ABC sampler using

```
1 $ run_ABC_NumCosmo.py -i <input_file>
```

¹¹In our case, $L = 2$, for observed features ξ and redshift.

¹²The number of quantiles is defined by the user in the input file, through the keyword `quantile_nodes`.

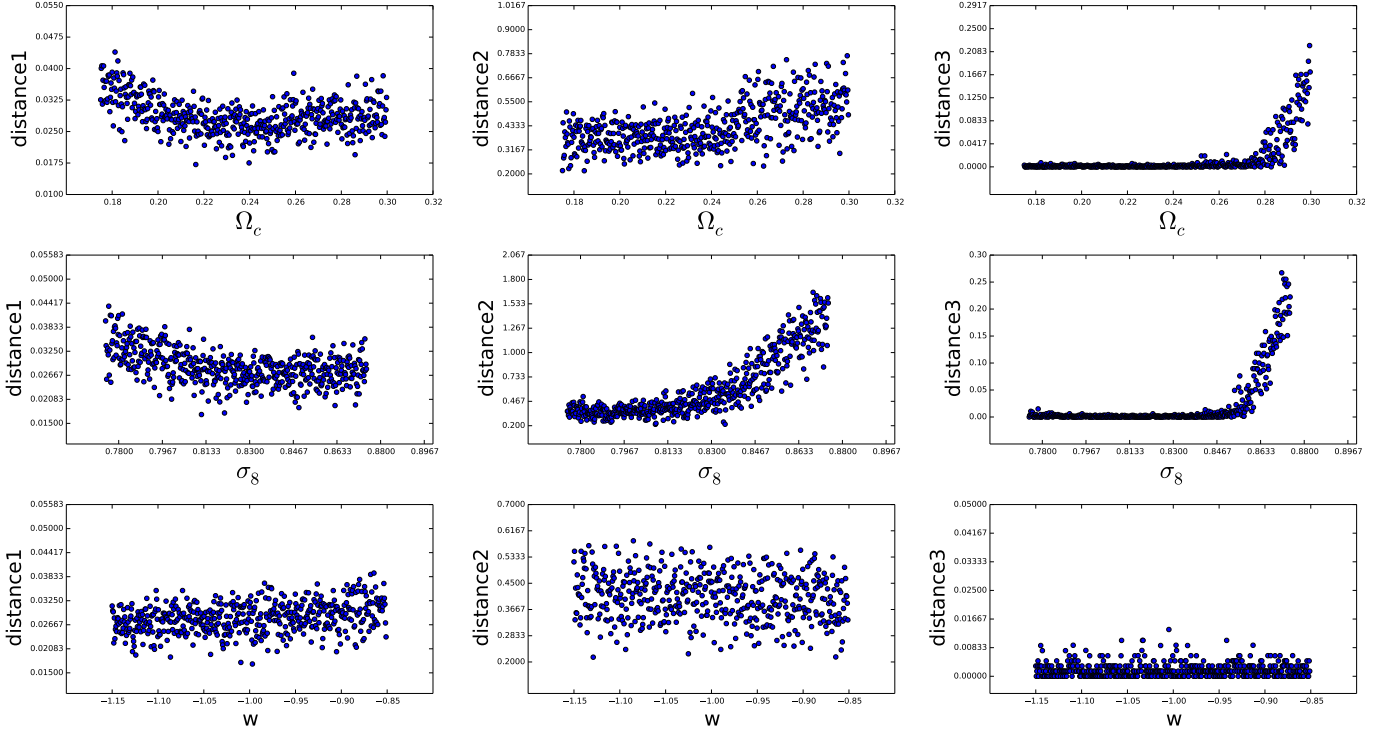


Figure 3: Behaviour of the quantile distance function in the context of galaxy clusters number counts. Each panel illustrates how the elements of the quantile based distance vary as a function of the cosmological parameters for 10⁴ random draws from the prior. Lines run through parameters and columns through distance elements.

Analogously, if the user is interested in continuing the calculations from a given particle system T on, this can be done using

```
1 $ continue_ABC_NumCosmo.py
2     -i <input_file>
3     -p T
```

In case a user defined distance or prior is chosen, it is necessary to include the `-f` option followed by the name of the function file in both examples above. Plots can be generated as shown in section 3.2.

Credible intervals from the ABC-PMC estimated posterior distributions are shown in Figure 4. The upper panels show 2-dimensions posteriors over the free parameters and the bottom panels display the profile of each parameter individually. Frames show the evolution of the approximated posteriors for consecutive particle systems. The first frame merely represents the initial prior: a flat PDF over all the free parameters. The next frame displays results from the first particle system ($t = 0$), where we generate a large number of simulations ($M = 50000$) and kept

only the 10% with smaller distance. From $t = 1$ on we clearly see how the posterior evolves and adapts through subsequent iterations. The credible intervals not only shrink, but also become asymptotically well behaved for further particle systems.

Worth noting, for this example each particle system holds $N = 5000$ particles and the convergence was achieved in 9 iterations for $\delta = 0.01$. In case a tighter posterior is desirable for Ω_c and σ_8 , one can simply decrease the convergence criteria, letting the system evolve for a little longer. If further information on w is desired, a more informative distance definition should also be used¹³ (see Figure 3). The evolution of the distance threshold and convergence criteria are shown in Figures 5 and 6, respectively.

¹³The quantile distance was chosen due to its simplicity and low computational cost. `cosmoabc` also contains a distance definition (Appendix B) which accounts for potential correlations between two parameters in a catalogue. We advise the user to consider the GRBF distance as well as the combination with other cosmological probes in case tight intervals over w are desired.

Figure 4: Results from coupling COSMOABC to the NUMCOSMO simulator. Use the control bottoms to display the evolution of particle systems. Frames run from successive iterations of the PMC-ABC algorithm. **Upper panel:** two-dimensional representation of the ABC posteriors in each iteration. **Lower left panel:** evolution of the dark matter density profile. **Lower centre panel:** evolution of the posterior over σ_8 . **Lower right panel:** evolution of the PDF profile over the dark energy equation of state parameter.

5. Final remarks

We presented COSMOABC, a Python implementation of Population Monte Carlo Approximate Bayesian Computation (PMC-ABC) algorithm with adaptive importance sampling. Traditional methods of parameter inference are useful if the likelihood is available and feasible to compute. Due to the increasing amount of data and their complex modelling in all areas of astronomy and cosmology, more and more computational power is required in order to explore larger parameter spaces whose internal correlations can often be impractically complicated or unknown. Thus, obtaining a statistical tool which bypasses the need of fully evaluating the likelihood is imperative. PMC-ABC presents an interesting alternative. cos-

MOABC is the first such implementation targeted to the astronomy and cosmology community.

The cosmological simulations are done through a connection with the *Numerical Cosmology* library (NUMCOSMO), but the code is flexible enough for user-specified distance, simulation and prior functions.

We stress that ABC is not a substitute for standard MCMC algorithms when the likelihood is completely known or easy to calculate. It is a viable alternative when we are not able to handle the likelihood itself, and thus in situations where a MCMC is not feasible.

In this work, we demonstrated the power of COSMOABC in estimating posterior probability distributions in two situations: a simple toy model and a complex cosmological simulation of a Sunyaev-Zeldovich sur-

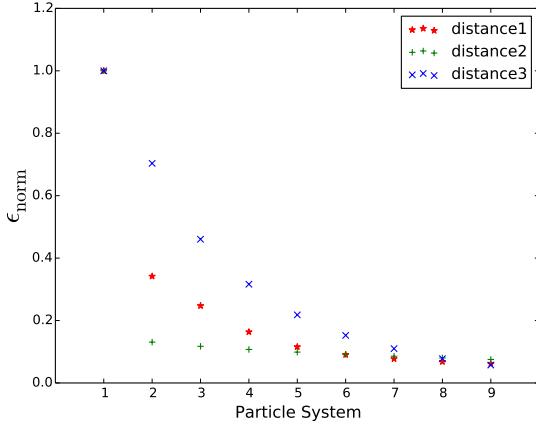


Figure 5: Evolution of the distance threshold. The first (stars), second (+) and third (x) elements of the quantile distance function were normalized by their respective larger values. The horizontal axis runs through all the particle systems shown in Figure 4.

vey. In both cases, we demonstrated how COSMOABC allows a good approximation of the true posterior probability distribution with a fairly simple and user-friendly interface. We used a completely synthetic environment in order to demonstrate the efficiency of the method and to be able to address the accuracy of the results. We hope this will be useful not only to cosmologists, but to all research areas in astronomy where simulations are becoming increasingly more accessible and systematics are making likelihood functions even more intractable.

The code is published under GPLv3 in PyPI and Github and documentation can be found in Readthedocs¹⁴.

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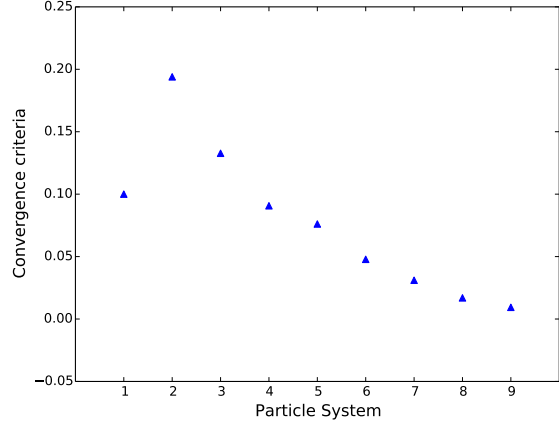


Figure 6: Evolution of the convergence criteria for results shown in figure 4.

moststatistics Initiative (COIN)¹⁵ is a non-profit organization whose aim is to nourish the synergy between astrophysics, cosmology, statistics and machine learning communities. This work was partially supported by the ESA VA4D project (AO 1-6740/11/F/MOS). EEOI is partially supported by the Brazilian agency CAPES (grant number 9229-13-2). SDPV is supported by CAPES (grant number 2649-13-6). MPL acknowledges the Brazilian agency CNPq (PCI/MC-TI/INPE program and grant number 202131/2014-9) for financial support. VCB was supported by CNPq-Brazil, with a fellowship within the program Science without Borders, FAPESP (grant number 2014/21098-1) and CAPES. AMMT was supported by the FCT/IDPASC grant number SFRH/BD/51647/2011.

Work on this paper has substantially benefited from using the collaborative website AWOB¹⁶ developed and maintained by the Max-Planck Institute for Astrophysics and the Max-Planck Digital Library. This work was written on the collaborative Overleaf platform¹⁷, and made use of the GitHub¹⁸ repository web-based hosting service and git version control software.

¹⁵<https://asaip.psu.edu/organizations/iaa/iaa-working-group-of-cosmostatistics>

¹⁶<http://awob.mpg.de>

¹⁷www.overleaf.com

¹⁸www.github.com

¹⁴<http://cosmoabc.readthedocs.org/en/latest/>

Appendix A. Cosmology with galaxy cluster number counts

The model assumes that the number density of halos with mass in the range $[M, M + dM]$ is strongly linked to both the matter-energy content of the Universe and the statistical properties of the initial linear density contrast field (Press & Schechter, 1974; Bond et al., 1991; Sheth & Tormen, 1999). Hence, the comoving number density of dark matter halos can be written as

$$\frac{dn(M, z)}{d \ln M} = -\frac{\rho_m(z)}{M} f(\sigma_R, z) \frac{1}{\sigma_R} \frac{d\sigma_R}{d \ln M}, \quad (\text{A.1})$$

where $\rho_m(z)$ is the mean matter density at redshift z , $f(\sigma_R, z)$ is the multiplicity function (Tinker et al., 2008), and σ_R^2 is the variance of the linear density contrast filtered on the length scale R ,

$$\sigma_R^2(z) = \int_0^\infty \frac{dk}{2\pi^2} k^2 P(k, z) |W(k, R)|^2, \quad (\text{A.2})$$

with a spherical top-hat window function, $W(k, R)$, and the linear power spectrum given by

$$P(k, z) = A k^{n_s} T(k)^2 D(z)^2. \quad (\text{A.3})$$

In the expression above the power spectrum depends on the spectral index, n_s , the linear growth function, $D(z)$, normalized such that $D(0) = 1$, and on the transfer function, $T(k)$ (Eisenstein & Hu, 1998). The normalization factor is written as

$$A = \frac{\sigma_8^2}{\int_0^\infty \frac{dk}{2\pi^2} k^{(n_s+2)} T(k)^2 W^2(k, 8)}. \quad (\text{A.4})$$

In order to obtain the mean number of DM halos with mass in the range $[M, M + dM]$ and in the redshift interval $[z, z + dz]$, we combine the mass function with the comoving volume element dV/dz , namely,

$$\frac{d^2 N}{dz d \ln M} dz d \ln M = \frac{dV}{dz} \frac{dn(M, z)}{d \ln M} dz d \ln M. \quad (\text{A.5})$$

Assuming a flat universe,

$$\frac{dV}{dz} = \Delta\Omega \left(\frac{\pi}{180} \right)^2 \frac{c}{H(z)} \left(\int_0^z dz' \frac{c}{H(z')} \right)^2, \quad (\text{A.6})$$

where $\Delta\Omega$ is the survey area in square degrees and $H(z)$ is the Hubble parameter

$$H(z) = H_0 [\Omega_m (1+z)^3 + (1 - \Omega_m) (1+z)^{3(1+w)}]^{1/2}, \quad (\text{A.7})$$

with Ω_m representing the fraction of total energy density in the form of matter (Ω_m), H_0 being the Hubble constant and w the equation of state of dark energy, considered to be constant.

This framework allows us to relate the mean number of DM halos within a certain range of mass and redshift (equation A.5) to the parameters describing the underlying cosmological model (equations A.1 to A.7). However, we still need to connect the theoretical redshift z and mass M with their equivalent observable quantities. We begin by taking into account the uncertainties from photometric redshift, z_{phot} , determination.

We assume that z_{phot} follows a Gaussian distribution with mean equal to z and standard deviation $\sigma = 0.05(1+z)$, which we refer to as $P(z_{phot}|z)$. Thus, the expected number of clusters for a given interval of z_{phot} and M can be written as,

$$\frac{d^2 N(M, z_{phot}, \theta)}{dz_{phot} d \ln M} = \int dz P(z_{phot}|z) \frac{d^2 N(M, z, \theta)}{dz d \ln M}, \quad (\text{A.8})$$

where θ comprises both the cosmological and astrophysical parameters (such as those of the mass-observable relation - see Appendix A.1).

Estimating the mass enclosed in a given galaxy cluster is not a trivial task (see e.g., Laganá et al., 2010; Giodini et al., 2013, and references therein). Traditionally, one requires the recognition of indirect signatures carrying such information into observable quantities, such as optical and X-ray emissions (Birkinshaw, 1999; Carlstrom et al., 2002). In particular, we use a mass-observable relation derived by the SPT team, which relies on measurements of the SZ effect.

Appendix A.1. Cluster mass estimate from Sunyaev–Zeldovich effect

The intracluster medium (ICM) is a hot plasma which interacts with photons of the cosmic microwave background (CMB) via Compton scattering, causing a spectral distortion in the CMB radiation. This is known as the SZ effect. The integrated thermal SZ

flux, Y_{SZ} , is proportional to the total thermal energy of the ICM (Barbosa et al., 1996; Motl et al., 2005) and consequently it is possible to use the SZ distortions on the CMB to estimate the mass of the cluster.

Due to significant uncertainties in the direct determination of Y_{SZ} , we follow here the strategy reported by the SPT (Vanderlinde et al., 2010; Benson et al., 2013; Reichardt et al., 2013), where an unbiased estimator ζ of the detection significance (signal to noise ratio) ξ is used as a mass proxy. In this context, $\zeta = \sqrt{\langle \xi \rangle^2 - 3}$ and $\zeta \propto Y_{SZ}/N_{int}$, with N_{int} denoting the noise per resolution element or the integrated noise over several resolution elements for unresolved and resolved detections, respectively. Moreover, the adopted mass scaling relation is given by

$$\zeta = A_{SZ} \left(\frac{M_{500}}{3 \times 10^{14} M_{\odot} h^{-1}} \right)^{B_{SZ}} \left(\frac{E(z)}{E(0.6)} \right)^{C_{SZ}}, \quad (\text{A.9})$$

where $E(z) = H(z)/H_0$, $M_{500} = (4\pi/3) 500 \rho_{crit} R_{500}^3$, with $\rho_{crit} = 3H_0^2/8\pi G$ as the critical energy density, R_{500} the radius enclosing $500 \times \rho_{crit}$ at the cluster redshift, and the scaling relation parameters A_{SZ} (ζ -mass normalization), B_{SZ} (ζ -mass slope) and C_{SZ} (ζ -mass redshift evolution) can be determined concomitantly with the cosmological parameters. Finally, substituting the true mass by the unbiased estimator in equation A.8, the number of clusters with $\xi \in [\xi, \xi + d\xi]$ and $z_{phot} \in [z_{phot}, z_{phot} + dz_{phot}]$ can be expressed as

$$\begin{aligned} \frac{d^2 N(\xi, z_{phot}, \theta)}{dz_{phot} d\xi} &= \int dz P(z_{phot}|z) \\ &\int d \ln M \int d\zeta \frac{d^2 N(M, z, \theta)}{dz d \ln M} \\ &P(\xi|\zeta) P(\ln \zeta | \ln M). \end{aligned} \quad (\text{A.10})$$

Following Benson et al. (2013), and Reichardt et al. (2013), we assume

$$\begin{aligned} P(\ln \zeta | \ln M) d \ln \zeta &= \frac{1}{\zeta \sqrt{2\pi} D_{SZ}} \times \\ &\exp \left[-\frac{(\ln \zeta - \ln M)^2}{2 D_{SZ}^2} \right] d\zeta, \end{aligned} \quad (\text{A.11})$$

with D_{SZ} being the log-normal scatter in ζ , and

$$P(\xi|\zeta) d\xi = \frac{1}{\sqrt{2\pi}} \exp \left[-\frac{(\xi - \sqrt{\zeta^2 + 3})^2}{2} \right] d\xi. \quad (\text{A.12})$$

Appendix B. Distance based on Gaussian Radial Basis Function

We describe bellow a distance defined in terms of Gaussian radial basis functions (GRBF), ρ_{GRBF} (within COSMOABC the function is called `distance_GRBF`). This is not a distance in the mathematical sense, since $\rho_{GRBF}(\mathcal{D}, \mathcal{D}_S) \neq \rho_{GRBF}(\mathcal{D}_S, \mathcal{D})$, but as the PMC-ABC is centred in the observed catalogue, it is enough to guide the sampler to the correct posterior distribution over the evolution of particle systems.

For a given simulated sample, we compute the approximation of its underlying model using a GRBF interpolation (Tsybakov, 2008),

$$G_R(\xi, z|\mathcal{D}) = \sum_{i=1}^{N_{sim}} \frac{1}{2\pi \sqrt{\det(\mathbf{C})}} \exp \left(-\frac{\mathbf{d}_i^T \cdot \mathbf{C}^{-1} \cdot \mathbf{d}_i}{2} \right), \quad (\text{B.1})$$

where

$$\begin{aligned} \mathbf{d}_i &= (\xi - \xi_{\mathcal{D}_S}^i, z - z_{\mathcal{D}_S}^i), \\ \mathbf{C} &= s^2 \text{cov}(\mathcal{D}), \end{aligned}$$

s is a scale parameter and $\text{cov}(\mathcal{D})$ is the covariance matrix of the observed data. Each element of the sum in equation (B.1) works as a kernel density distribution centred in the i -th simulated cluster with (ξ_i, z_i) . Consequently, $G_R(\xi_*, z_*)$ is the number of clusters we expect to observe having (ξ_*, z_*) .

We can re-obtain the total number of objects in the catalogue through

$$\int d\xi \int dz G_R(\xi, z|\mathcal{D}) = N_{sim}. \quad (\text{B.2})$$

Making use of the auxiliary function

$$\ln f(\mathcal{D}|\mathcal{D}_S) = \sum_{j=1}^N \ln(G_R(z_j, \xi_j|\mathcal{D}_S)) - N_{sim}, \quad (\text{B.3})$$

with the index j running through all the data points in \mathcal{D} (Penna-Lima et al., 2014), the distance between the “observed” and simulated catalogues is given by

$$\rho(\mathcal{D}, \mathcal{D}_s) = -2 \ln \left(\frac{f(\mathcal{D}|\mathcal{D}_s)}{f(\mathcal{D}|\mathcal{D})} \right). \quad (\text{B.4})$$

Therefore, in each iteration, t , we will only accept those parameter values whose forward model satisfy $\rho_t(\mathcal{D}, \mathcal{D}_s) \leq \epsilon_t$ and the ABC-PMC algorithm can be employed normally¹⁹.

The scale parameter s (equation B.2) regulates our tolerance towards distinct distributions which produce the same total number of objects in a catalogue. Suppose we begin with a large ϵ_1 and follow the ABC-PMC algorithm reducing ϵ_t at each time-step. If s is too small the probability of finding parameter values satisfying the distance threshold will drop steadily, rendering the algorithm unable to further reduce ϵ_t . On the other hand, if s is too large, the density function will evolve to a very flat behaviour losing all information about the underlying distribution of \mathcal{D} . Thus, s must be chosen such that most of the shape information in \mathcal{D} is retained, while still being feasible to reduce ϵ_t until the desired precision is achieved. For the specific case outlined here, we found that any $s \in [0.1, 0.5]$ will lead to well constrained and unbiased results.

In order to call this distance definition from within cosmoABC, the input file must include the extra parameter s and the function definition

```
1 ...
2 distance_func = distance_GRBF
3 s = 0.15
4 ...
```

The GRBF distance is more time consuming, since it takes into account the correlation between the observed features. However, it might be worth to use it in highly correlated data scenarios. The current version of the NUMCOSMO library includes an ABC sampler using the GRBF distance.

¹⁹Note that the denominator in equation B.4 is a scalar independent of the mock data. This ensures the distance function convergence.

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